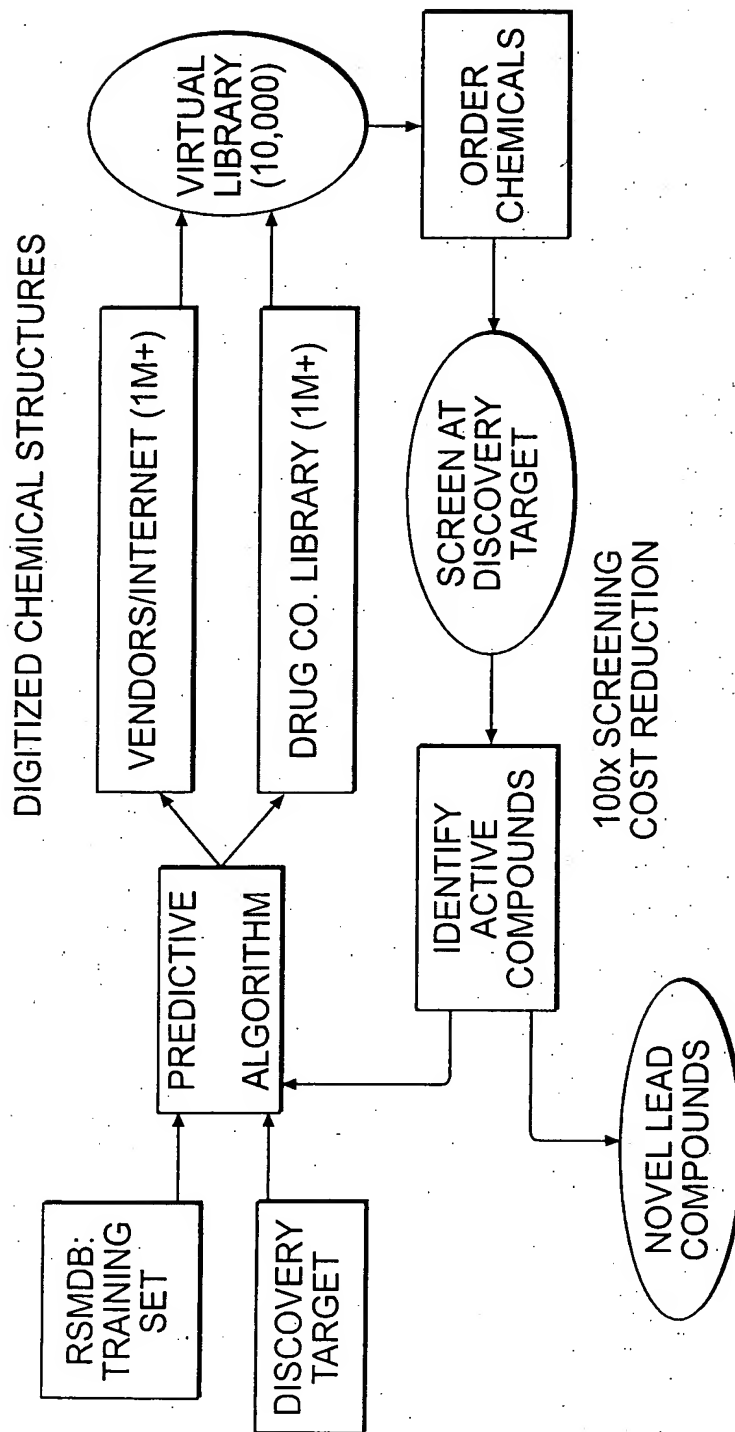


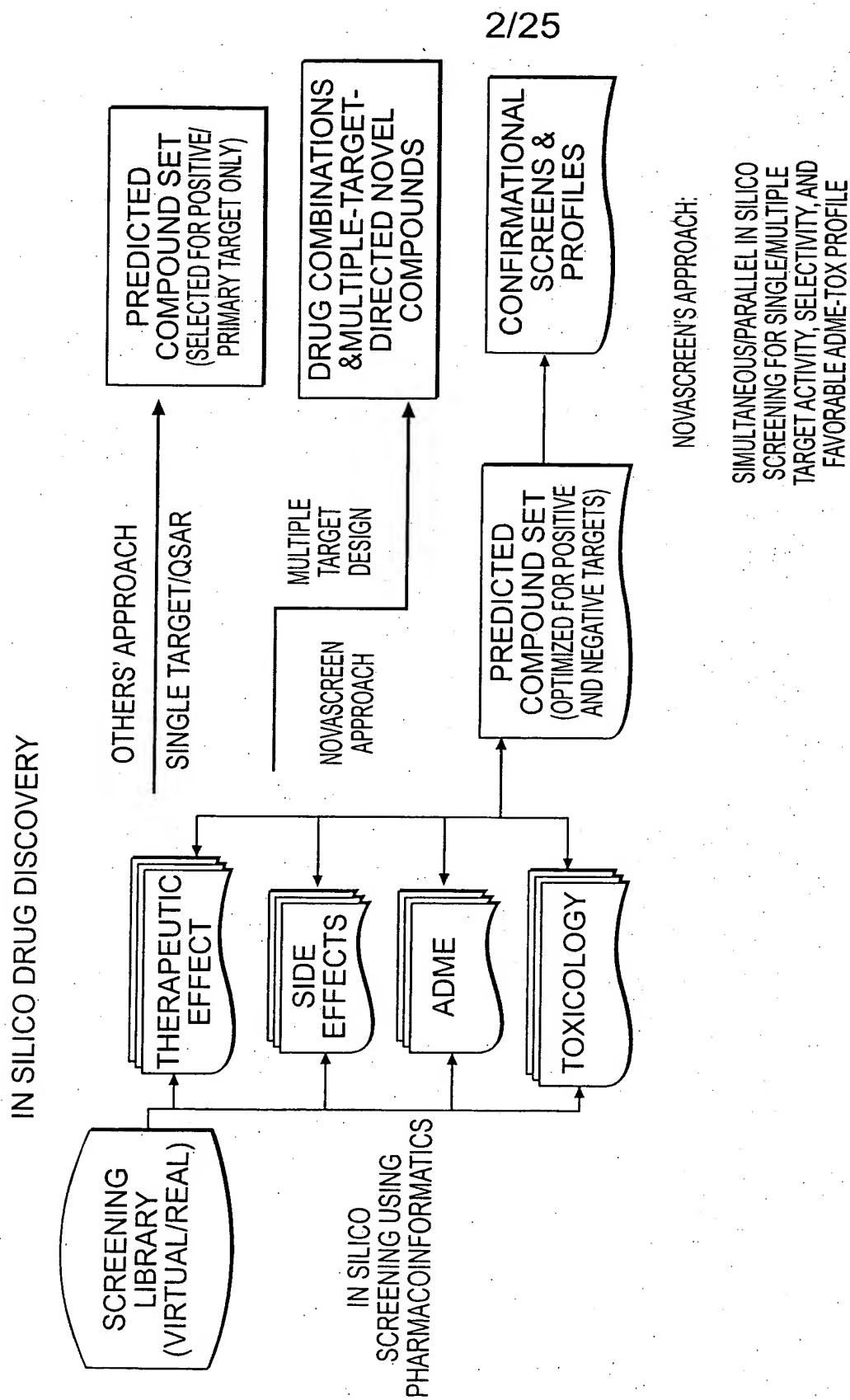


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# PHARMACOAinformatics FOR DRUG DISCOVERY



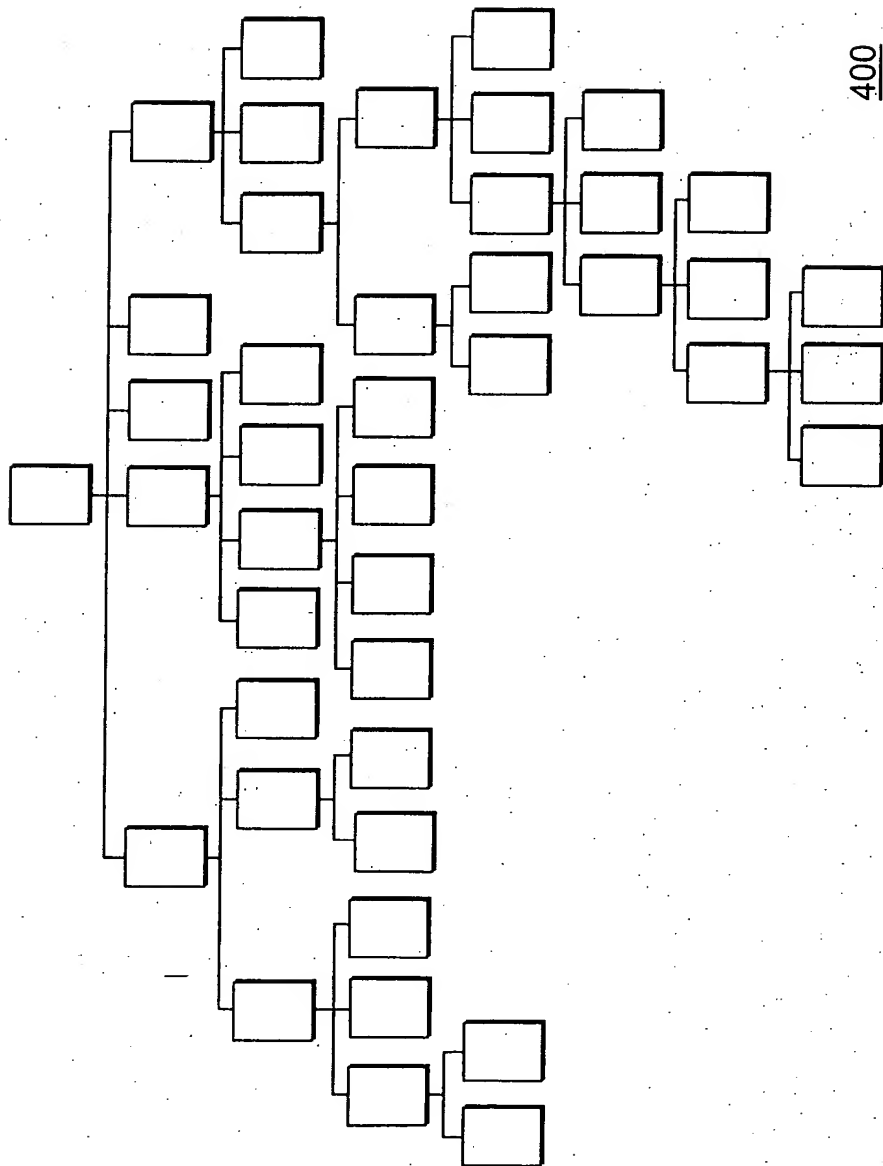
**FIG. 1**



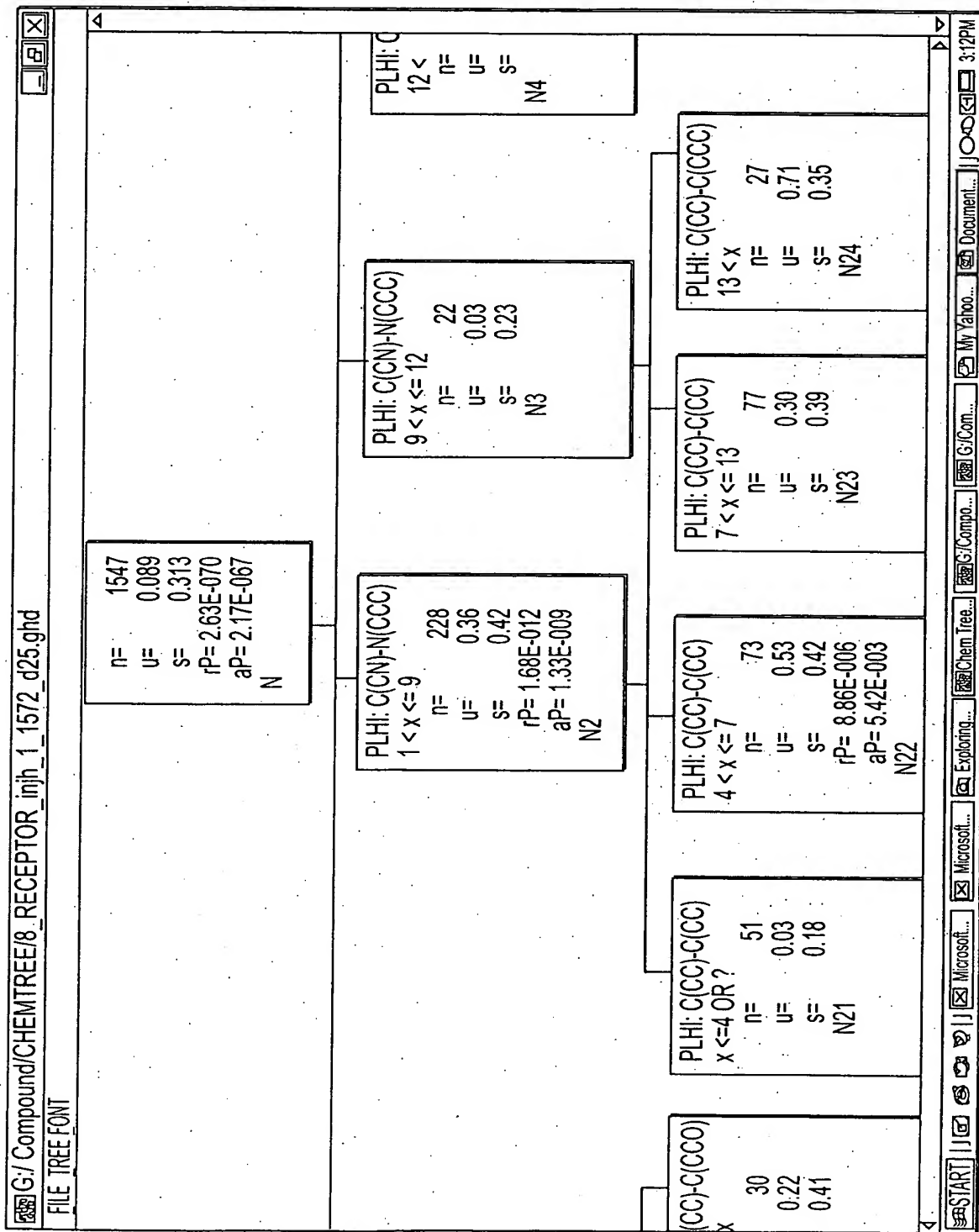
**FIG. 2**

$$\begin{aligned}
 \Sigma P_T &= \Sigma P_D + \Sigma P_{UD} \\
 \Sigma P_D &= \Sigma P_{prot\_1} + \Sigma P_{prot\_2} + \dots + \Sigma P_{phys\_1} + \Sigma P_{phys\_2} + \Sigma P_{phys\_n} \dots \\
 \Sigma P_{UD} &= \Sigma P_{prot\_1_u} + \Sigma P_{prot\_2_u} + \dots + \Sigma P_{phys\_1_u} + \Sigma P_{phys\_2_u} + \Sigma P_{phys\_n_u} \dots
 \end{aligned}$$

**FIG. 3**



**FIG. 4**



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- PLHI: N(CC) - N(CC) X = 3
  - PLLO: C(CCC) - N(CC) X = 2
  - PLHI: C(CCC) - N(CC) X = 5
  - PLLO: C(CNN) - N(CC) X = 1
  - PLHI: C(CNN) - N(CC) X = 2

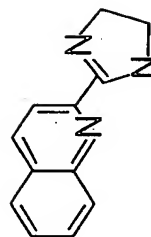


FIG. 6

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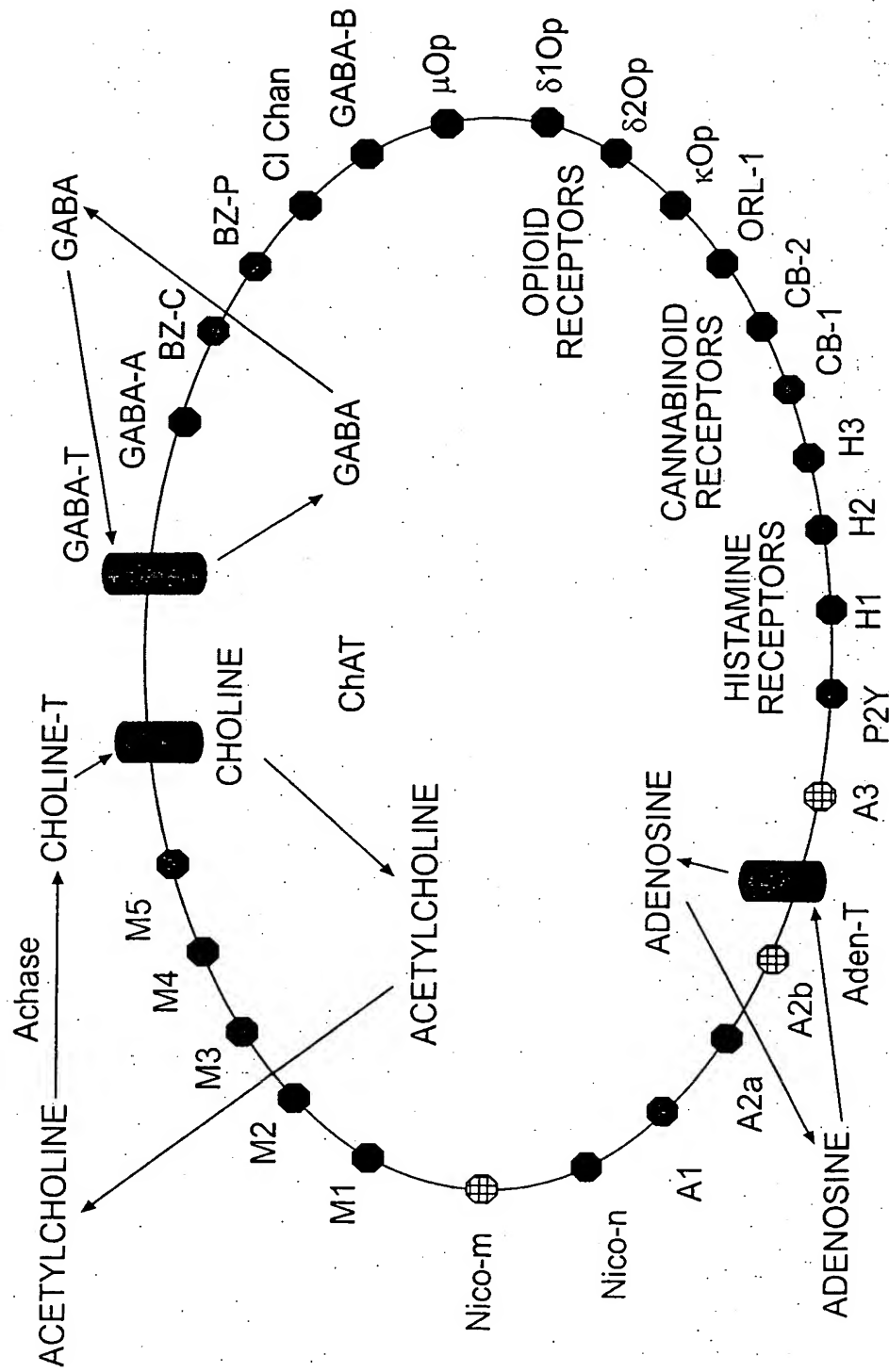


FIG. 7



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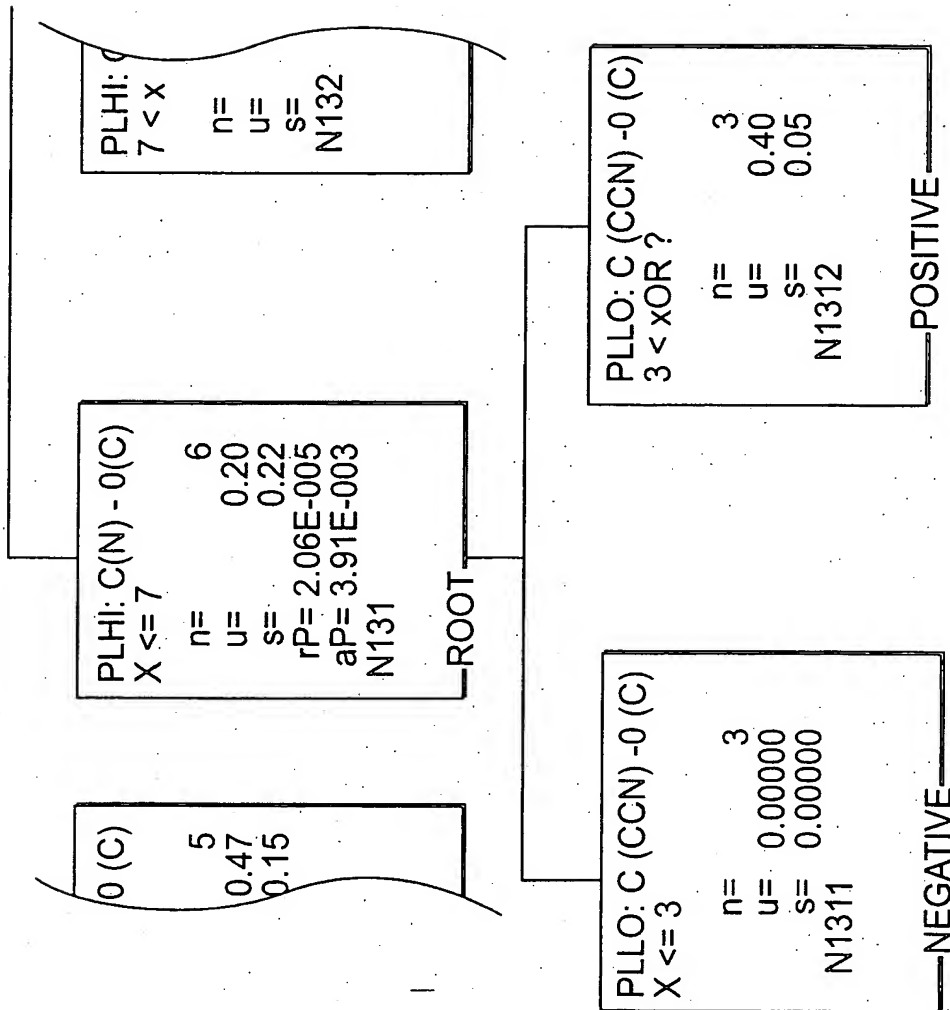
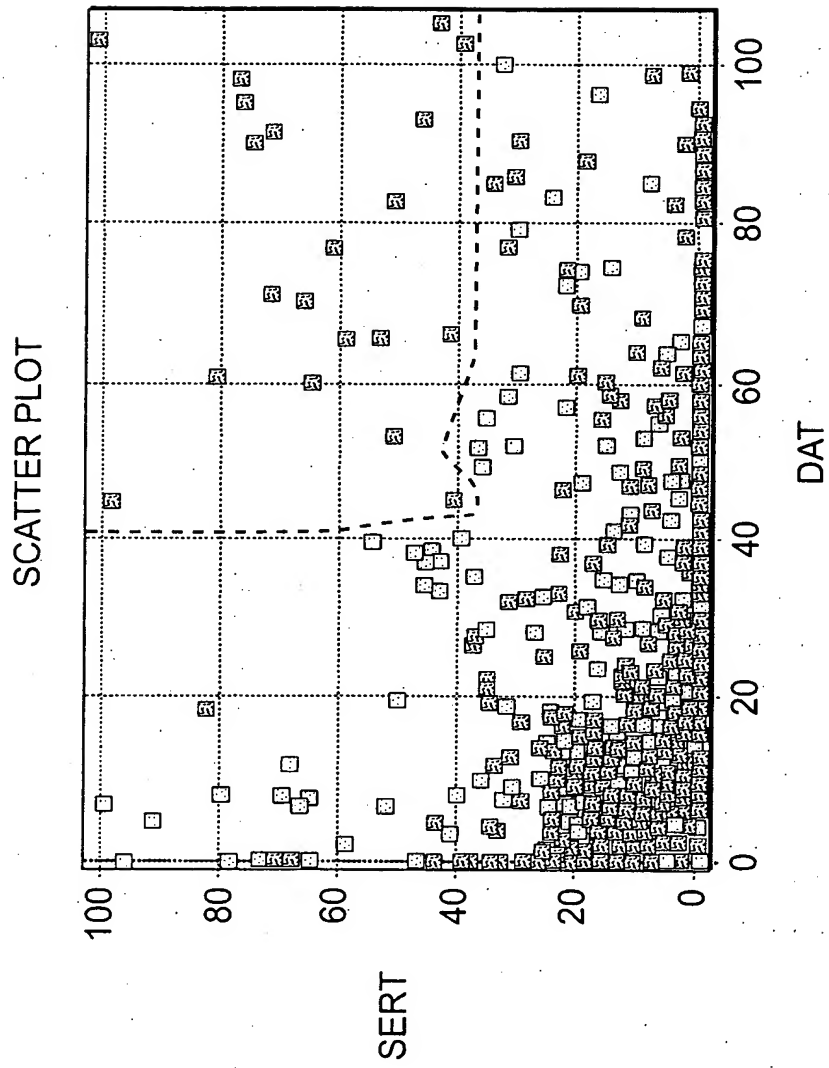


FIG. 9

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**FIG. 10**

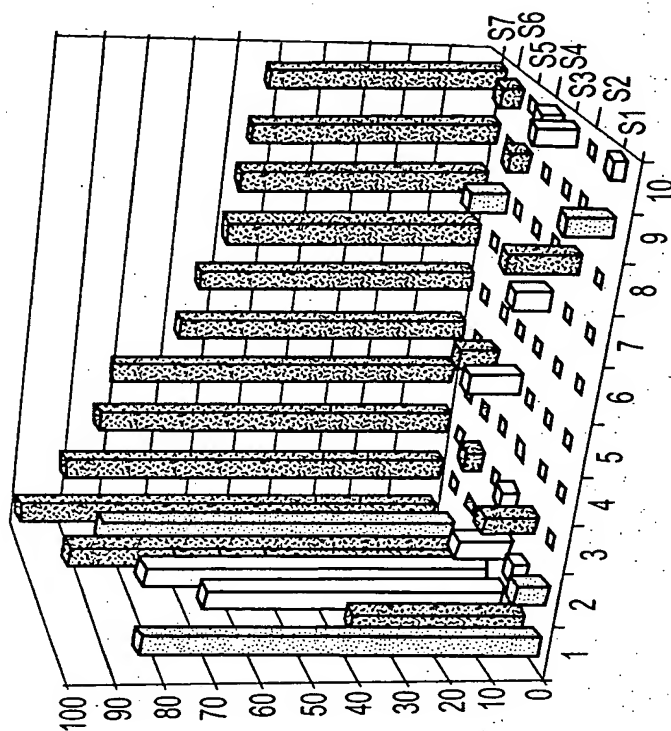
PHARMACoinformatics  
SINGLE STEP APPROACH TO OPTIMIZED LEADS

AN EXAMPLE OF FINDING BETTER AND CLEANER DRUG CANDIDATES

IN SILICO SCREEN 240,000 CMPDS

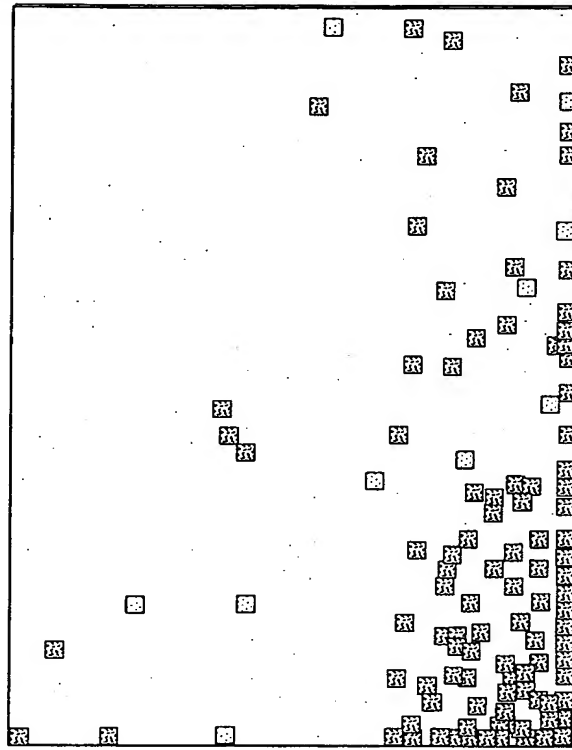
- 400 COMPOUNDS
- 34 HITS
- 5 STRUCTURAL CLASSES
- 9 HITS WITH DESIRED  
TARGET SPECIFICITY

CONFIDENTIAL

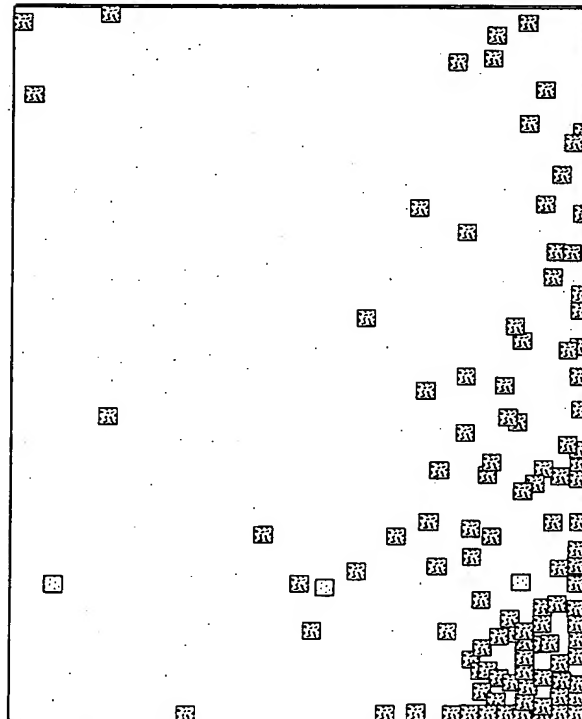


**FIG. 11**

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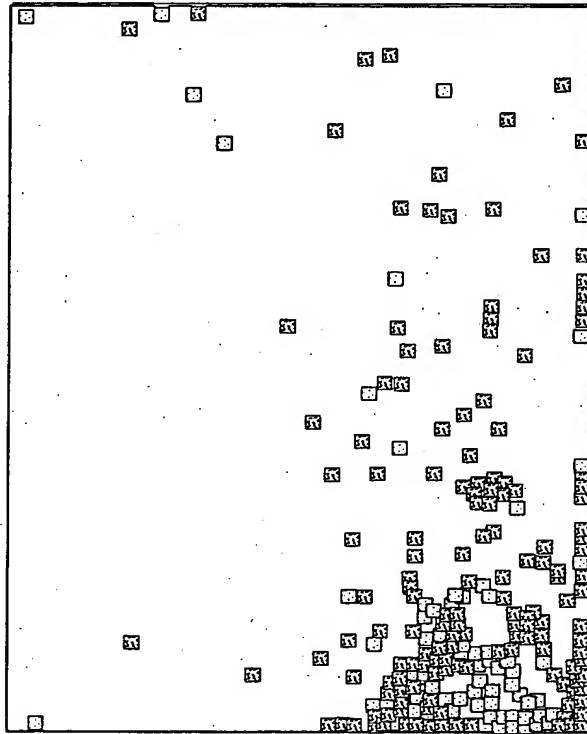


**FIG. 12b**

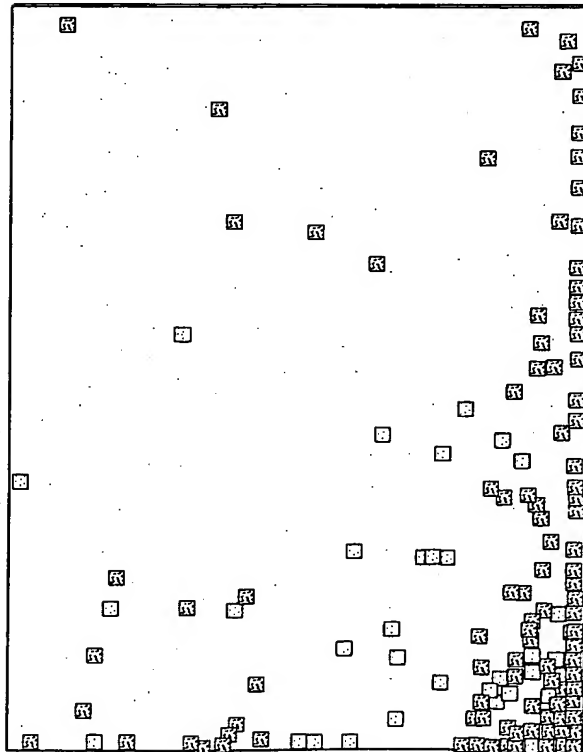


**FIG. 12a**

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**FIG. 12d**



**FIG. 12c**

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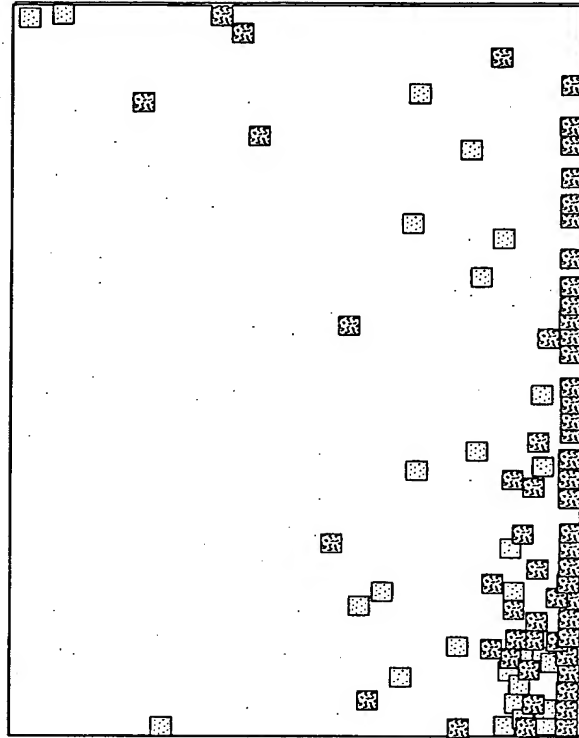


FIG. 12f

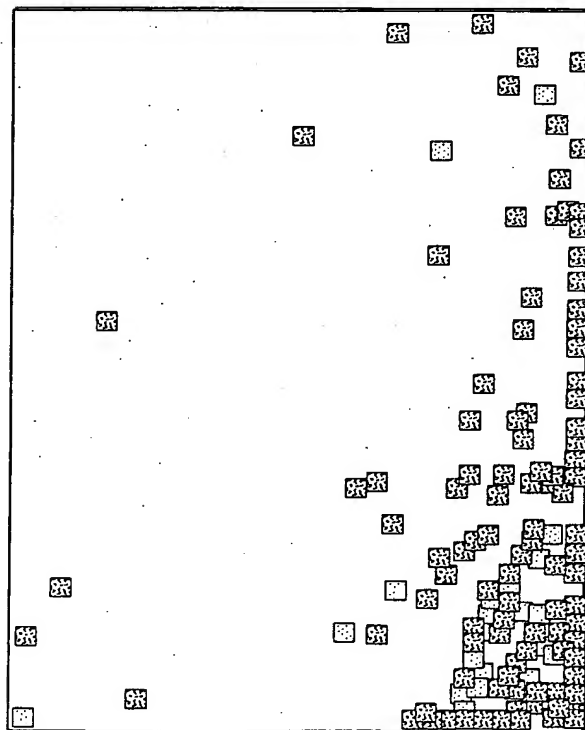
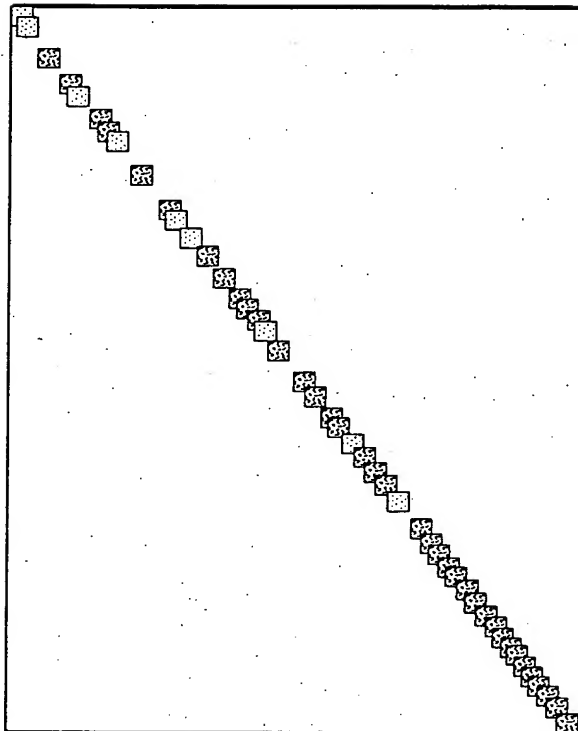
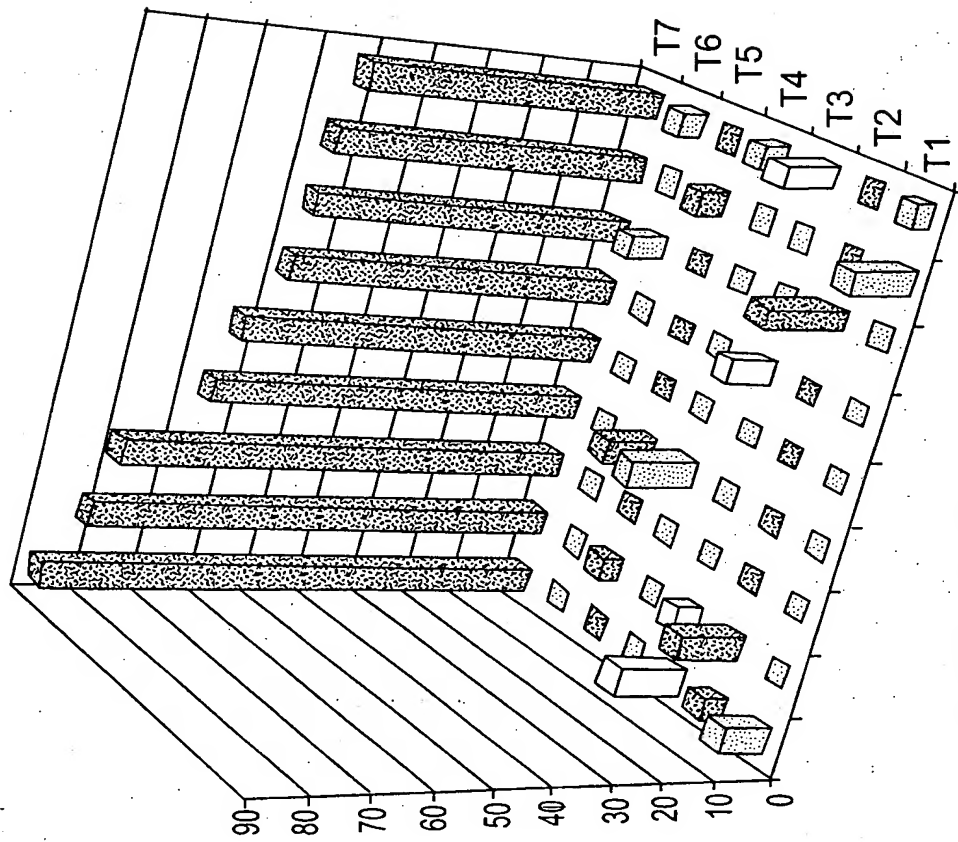


FIG. 12e



**FIG. 12g**



**FIG. 13**



A2A\_D1

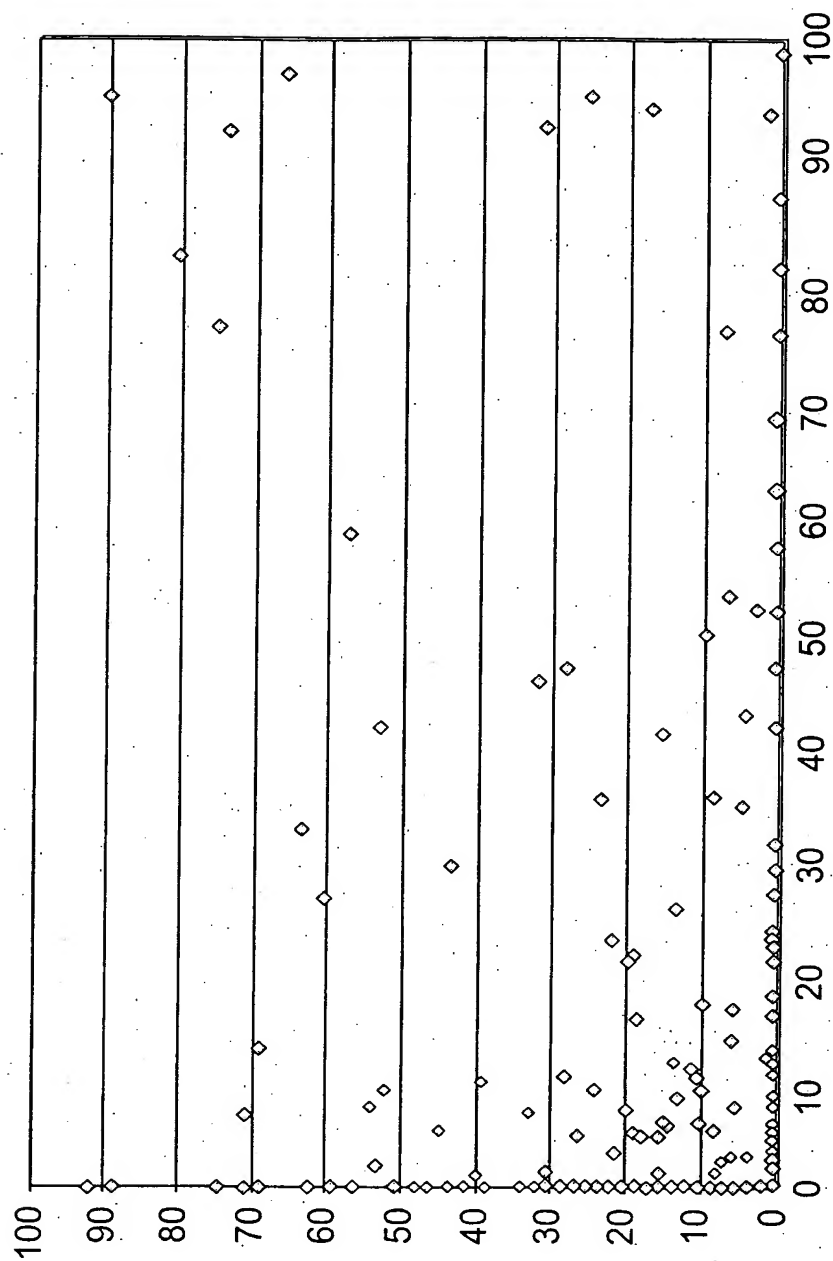


FIG. 14

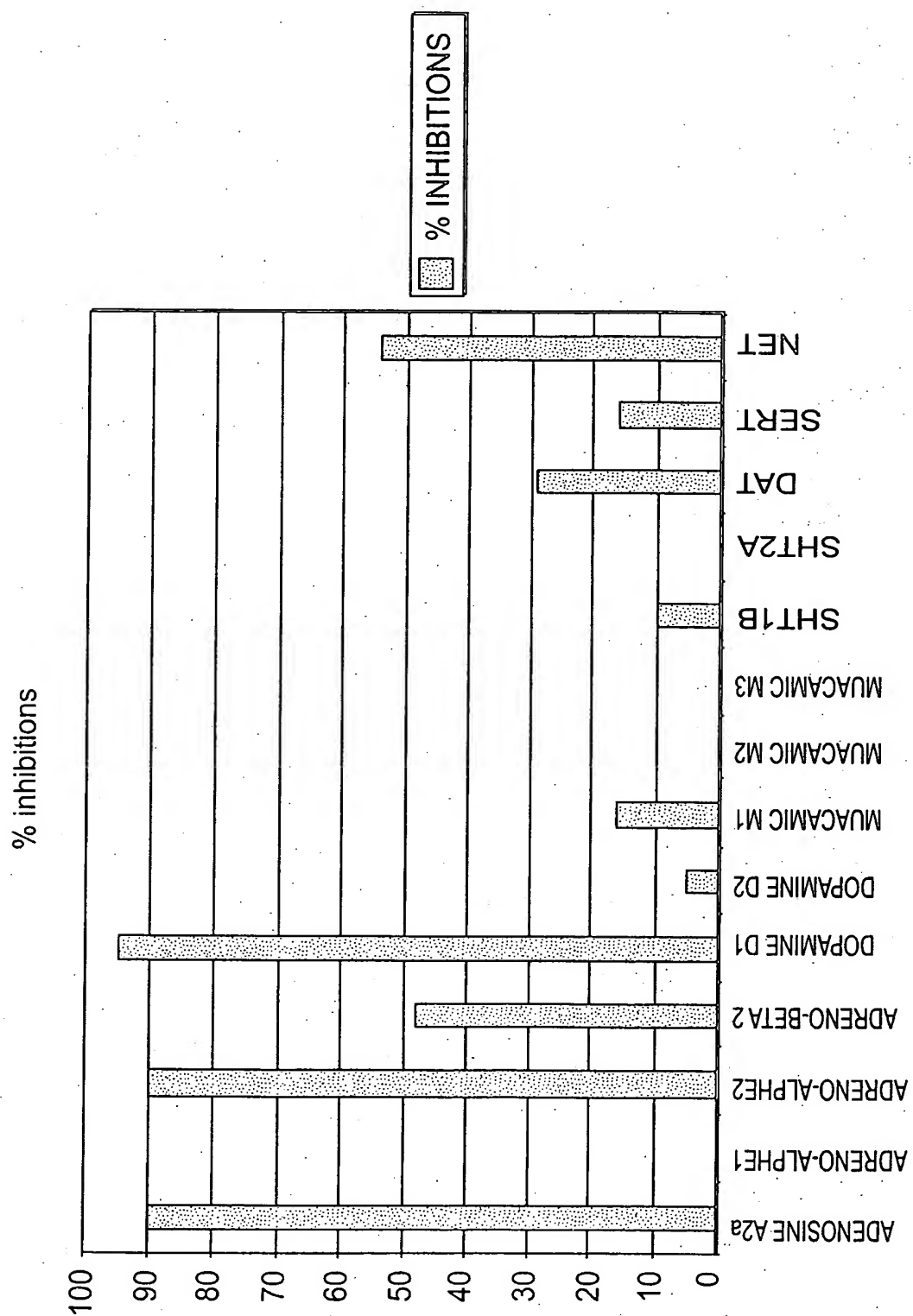


FIG. 15

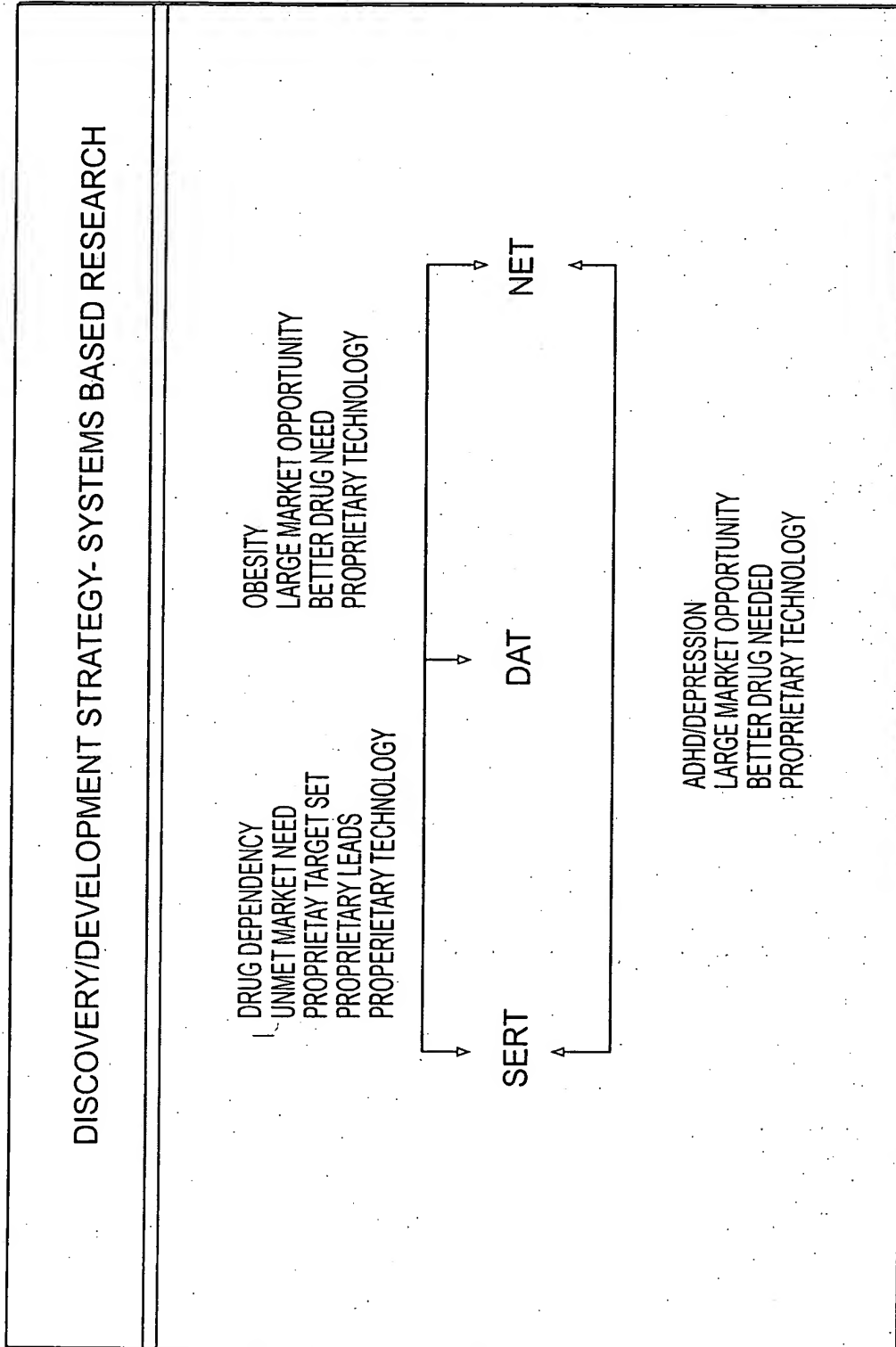
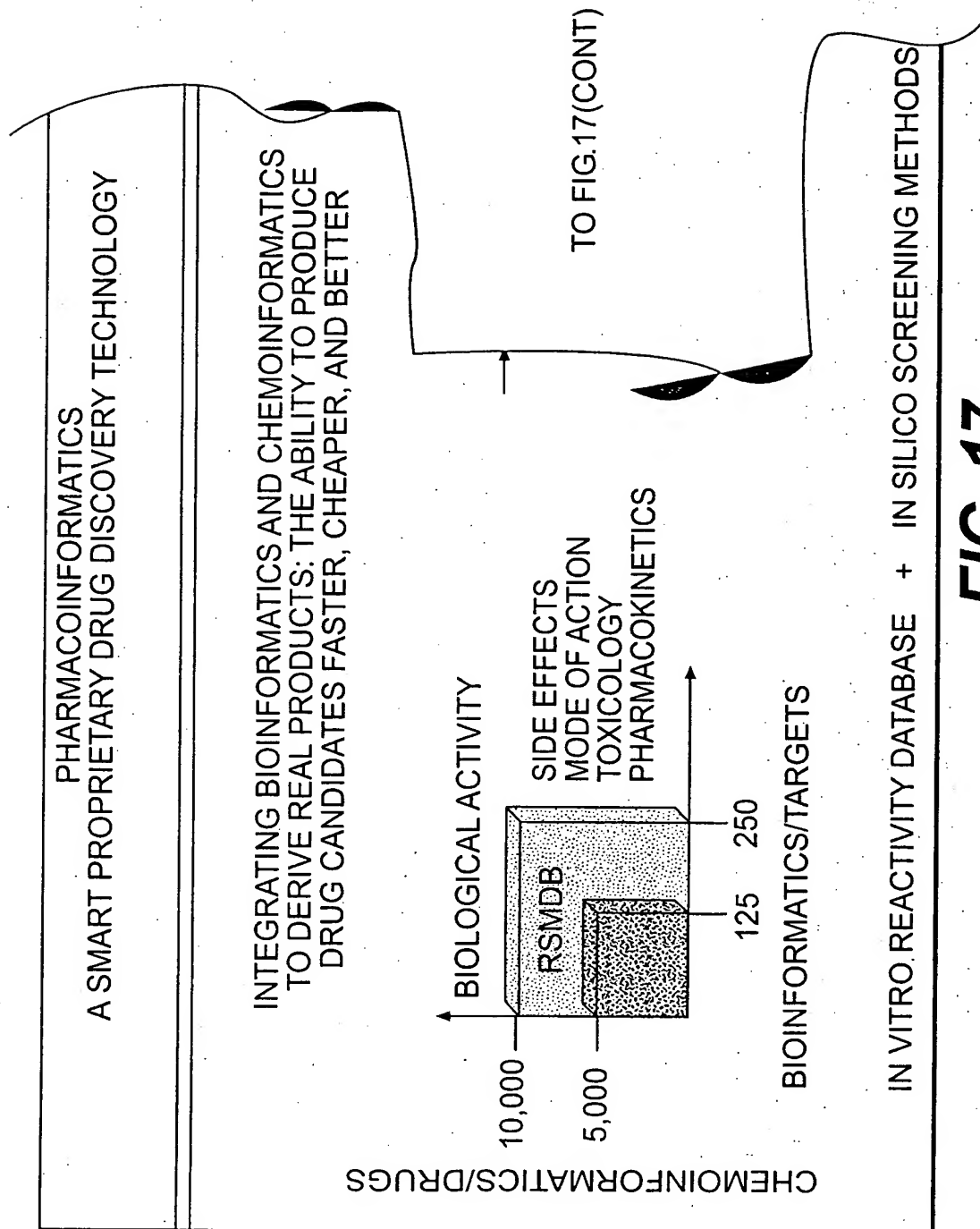
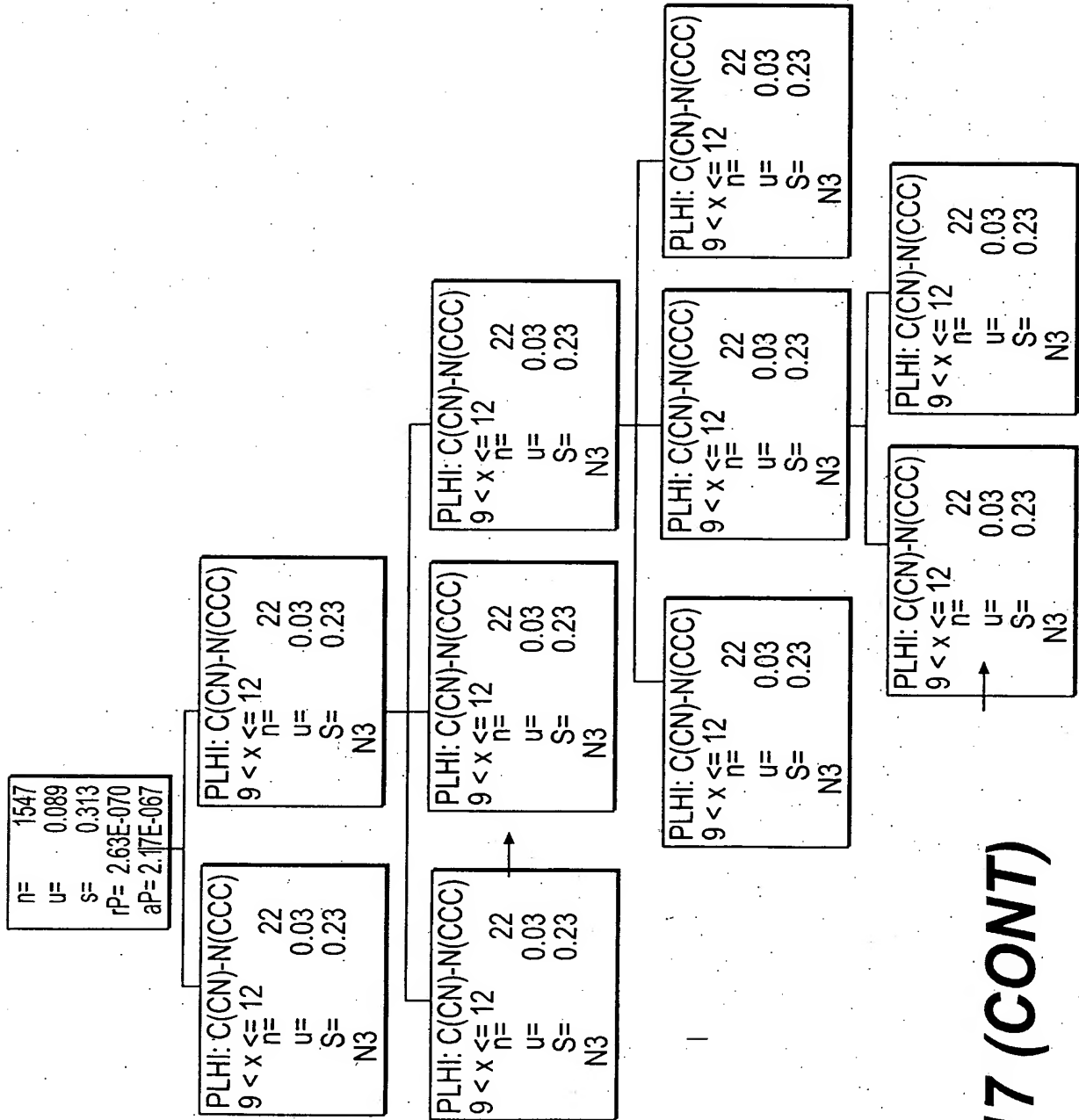


FIG. 16



**FIG. 17**



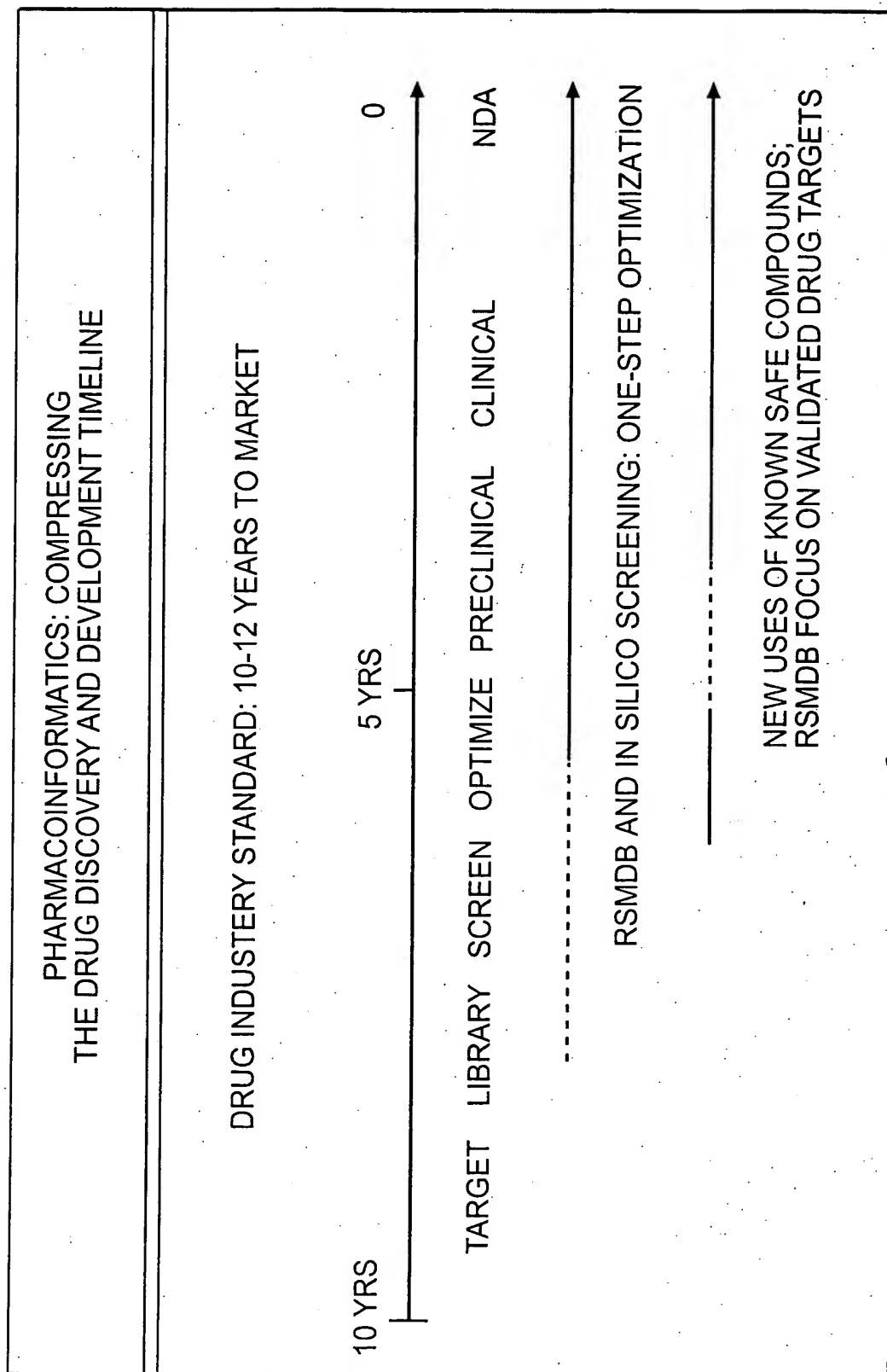
**FIG. 17 (CONT)**

RSMDB CONTENT: COMPOUND CLASSES
<ul style="list-style-type: none"><li>• PRESCRIPTION DRUGS (1500-2000)</li><li>• OTC MEDICINES; VETERINARY MEDICINES</li><li>• AGRICULTURAL/ENVIRONMENTAL CHEMICALS</li><li>• DRUGS IN CLINICAL TRIALS (&amp; LIKE STRUCTURES)</li><li>• DISCONTINUED/FAILED DRUG CANDIDATES (AND LIKE/SIMILARITY STRUCTURES)</li><li>• PHARMACOLOGICAL REFERENCE AGENTS</li><li>• BIOACTIVE NATURAL PRODUCTS</li><li>• + STRUCTURALLY DIVERSE CHEMICAL COMPOUNDS</li></ul>

**FIG. 18**

RSMDB CONTENT: TARGET CLASSES	
<ul style="list-style-type: none"><li>• DRUG DISCOVERY MOLECULAR TARGETS</li><li>• SIDE EFFECT TARGETS</li><li>• IN VITRO TOXICOLOGY TARGETS</li><li>• IN VITRO PHARMACOKINETIC TARGETS</li><li>• SELECTED FROM 300 AVAILABLE DEVELOPED ASSAYS</li></ul>	RECEPTORS
	ENZYMES
	TRANSPORTERS
	ION CHANNELS
ENRICHED SET OF MARKET-VALIDATED GPCR TARGETS, ESPECIALLY FOR CNS DISEASES	

**FIG. 19**



**FIG. 20**



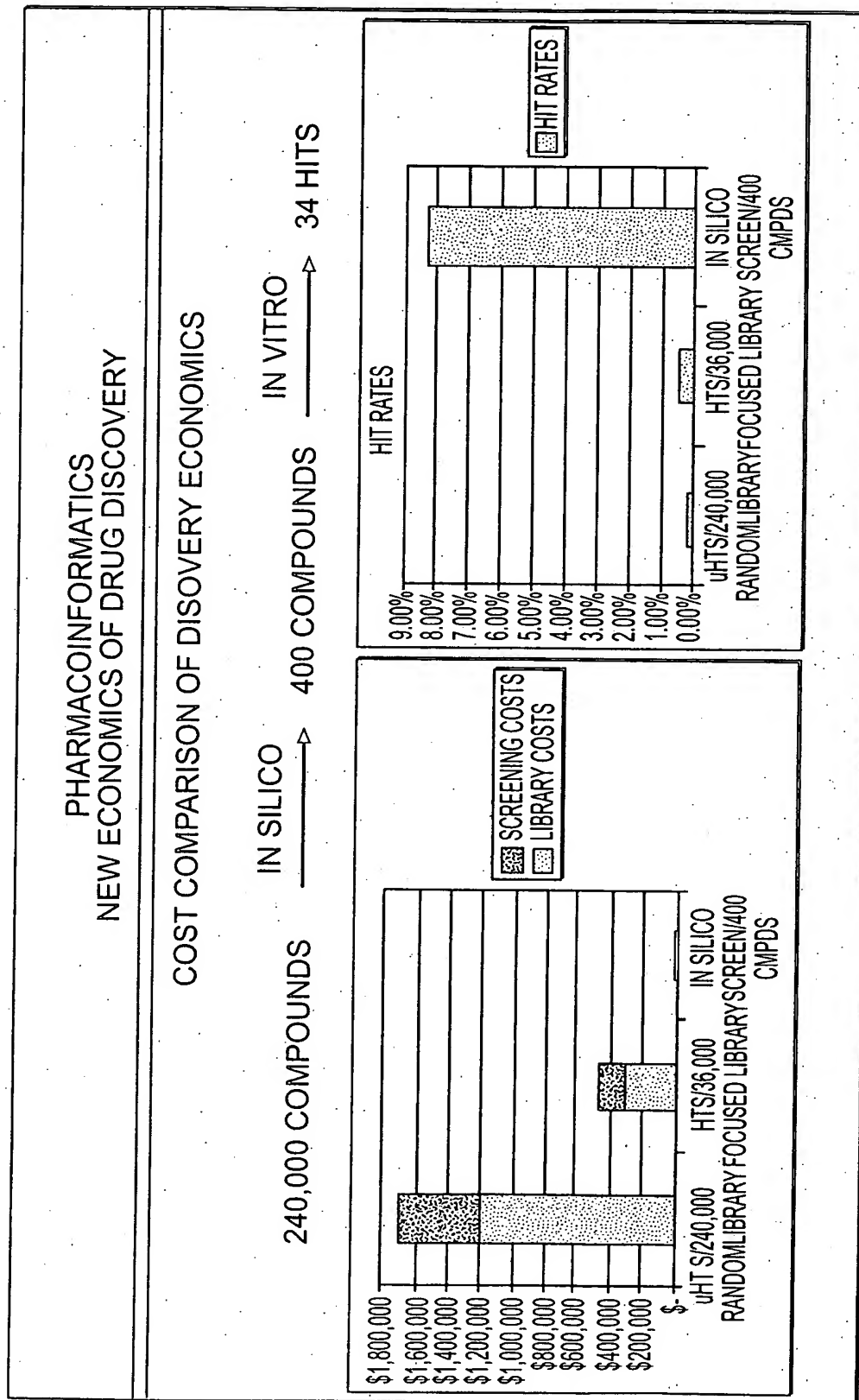


FIG. 21